

UCRL-94561
PREPRINT

THE Be-C (BERYLLIUM-CARBON) SYSTEM

H. Okamoto
L. E. Tanner

CIRCULATION COPY
SUBJECT TO RECALL
IN TWO WEEKS

This paper was prepared for submittal to
Bulletin of Alloy Phase Diagrams

April 29, 1986

Lawrence
Livermore
National
Laboratory

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial products, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

The Be-C (Beryllium-Carbon) System
9.01218 12.011

By H. Okamoto and L.E. Tanner
Lawrence Livermore National Laboratory

Equilibrium Diagram

The Be-C system has been reviewed repeatedly, e.g., by [1899Leb], [52Cool], [58Pas], [60Beal], [63Fral], [63Sch], [64Evel], [72Ald], [73Fer], and [73Goll], as well as by [Hansen], [Elliott], and [Shunk]. However, the available information on the phase diagram has not advanced significantly from that presented in [Hansen].

Be_2C is the only stable compound; there has been speculation that BeC_2 exists as a metastable phase.

Be Terminal Phases. The melting point of βBe and the $\beta\text{Be} \rightarrow \alpha\text{Be}$ allotropic transformation temperature are 1289 ± 4 and 1270 ± 6 °C, respectively [86BAP]. The solubility of C in αBe appeared to be negligible according to the microstructural studies by [32Slo] and [50Kaul]. A similar study by [57Grel] bracketed the solubility of C to be less than 0.23 at.%. The actual solubility seems to be even lower. This is suggested by the self-diffusion of Be, which may be explained only if the C content is extremely small (~ 0.5 ppm) [70Chal].

C Terminal Solid Solution. No information is available.

Be_2C Phase. This phase was first prepared by the direct reaction of a powder mixture of Be and C [1899Leb, 16Oes] at $T > 1300$ °C, or alternatively by the reaction $2\text{BeO} + 3\text{C} = \text{Be}_2\text{C} + 2\text{CO}$ [1895Leb, 15Fic, 51Gall] at $T > 1700$ °C. However, in more recent studies Be_2C has been found to decompose into $2\text{Be(g)} + \text{C(s)}$ at $T > 2150$ °C before reaching the melting point at ~ 2400 °C [53Mal, 54Mal, 55Quil]. The equilibrium pressure for this reaction was measured to be $\log P(\text{atm}) = 7.026 \pm 0.347 - (19720 \pm 5377)/T$ (°C) [59Poll] between 1157 and 1396 °C. This compound is also unstable in the presence of moisture at room temperature, forming Be(OH)_2 [52Cool]. Traces of Be_2C were also found on the electron-bombarded surface of Be in the presence of a hydrocarbon polymer [65Moll].

BeC_2 . The reaction of acetylene gas over Be powder at 450 °C appeared to form a compound with the probable formula BeC_2 [24Durl]. The Be acetylides is expected to transform into the stable Be_2C phase at higher temperatures, but this could not be confirmed [43Rue].

Crystal Structures

A summary of crystal structure data of the Be-C system is given in Table 1. The structure of Be_2C was identified as the CaF_2 -type by [31Sta, 34Sta]. The lattice parameter was also measured by the same authors to be 0.434 ± 1 nm, which was confirmed by [48Tei], [54Mall], [56Sta], and [66Mat]. The most accurate value was obtained by [56Sta]

and is given in Table 1.

Thermodynamics

The heat capacity of Be_2C is given by [50Neel] as $42.7 + 21.4 \times 10^{-3}T$ ($^\circ\text{C}$) J/mole K. The thermodynamic parameters (enthalpy and entropy of fusion, Gibbs energy) of Be_2C were measured and discussed by various investigators, viz [55Kri], [55Qui], [59Pol], [60NBS], [63Sch], [64Mot], [68Bl], [70Bl], and [80Kat]. Inconsistencies between the values given by earlier investigators and the observed stability of Be_2C were pointed out by [64Mot]. The assessed values by [72Ald] on the basis of the dissociation pressure of Be_2C [59Pol] and calorimetric data [70Bl] are $\Delta H_{298}^\circ = -117 \pm 0.8$ kJ/mol and $S_{298}^\circ = 16.3 \pm 4.6$ J/mol K.

Cited References

- *1895Leb: P. Lebeau, "Beryllium Carbide," Compt. Rend., **121**, 496-499 (1895) in French; Abstr. in J. Chem. Soc., **70**, part II, 169 (1896) in French. (Equi Diagram; Experimental)
- 1899Leb: P. Lebeau, "Researches on Beryllium and its Compounds," Ann. Chim. Phys., **16**, 457-503 (1899) in French. (Equi Diagram; Review)
- 15Fic: F. Fichter and E. Brunner, "Beryllium Nitride," Z. Anorg. Chem., **93**, 84-94 (1915) in German. (Equi Diagram; Experimental)
- 16Oes: G. Oesterheld, "Alloys of Beryllium with Aluminum, Copper, Silver and Iron," Z. Anorg. Chem., **97**, 6-40 (1916) in German. (Equi Diagram; Experimental)
- 24Dur: J.F. Durand, "Formation of Metallic Acetylides. II. Action of Acetylene on the Metals," Bull. Soc. Chim. France, **35**, 1141-1144 (1924) in French. (Equi Diagram; Experimental)
- *31Sta: M. v. Stackelberg, "The Crystal Structure of Several Carbides and Borides," Z. Elektrochem., **37**, 542-545 (1931) in German. (Crys Structure; Experimental)
- 32Slo: H.A. Sloman, "Researches on Beryllium," J. Inst. Metals, **49**, 365-388 (1932). (Equi Diagram; Experimental)
- 34Sta: M. v. Stackelberg and F. Quatram, "The Structure of Beryllium Carbide, Be_2C ," Z. Phys. Chem., **B27**, 50-52 (1934) in German. (Crys Structure; Experimental)
- 43Rue: W.H.C. Rueggeberg, "The Carbides of Magnesium," J. Am. Chem. Soc., **65**(4), 602 (1943). (Equi Diagram; Theory)
- 48Tei: R.J. Teitel, "The Beryllium-Iron System," U.S. At. Energy Comm., Publ. AECD-2251, **88** (1948). (Crys Structure; Experimental)

- 50Kau: A.R. Kaufmann, P. Gordon, and D.W. Lillie, "The Metallurgy of Beryllium," Trans. ASM, 42, 785-844 (1950). (Equi Diagram; Experimental)
- 50Nee: J.J. Neely, C.E. Teeter, Jr., and J.B. Trice, "Thermal Conductivity and Heat Capacity of Beryllium Carbide," J. Am. Ceram. Soc., 33(12), 363-364 (1950). (Thermo; Experimental)
- 51Gal: M. Gallagher, "New Analytical Developments," J. Southern Research, 3(4), 14-15 (1951). (Equi Diagram; Experimental)
- 52Coo: J.H. Coobs and W.J. Koshuba, "The Synthesis, Fabrication, and Properties of Beryllium Carbide," J. Electrochem. Soc., 99, 115-120 (1954). (Equi Diagram; Review)
- 53Mal: M.W. Mallett, E.A. Durbin, M.C. Udy, D.A. Vaughan, and E.J. Center, "Preparation and Examination of Beryllium Carbide," U.S. At. Energy Comm., Publ. BMI/MWM/5 (1953). (Equi Diagram; Experimental)
- *54Mal: M.W. Mallett, E.A. Durbin, M.C. Udy, D.A. Vaughan, and E.J. Center, "Preparation and Examination of Beryllium Carbide," J. Electrochem. Soc., 101, 298-305 (1954). (Equi Diagram, Crys Structure; Experimental)
- 55Kri: O.H. Krikorian, "High Temperature Studies; Part II, Thermodynamic Properties of the Carbides," U.S. At. Energy Comm., UCRL-2888 (1955). (Thermo; Experimental)
- 55Qui: J.F. Quirk, "Beryllium Carbide" in Reactor Handbook, vol. 3, Materials: U.S. At. Energy Comm. ABCD-3647, 95-106 (1955). (Equi Diagram, Thermo; Experimental)
- 56Sta: E. Staritzky, "Diberyllium Carbide, Be_2C ," Anal. Chem., 28, 915 (1956). (Crys Structure; Experimental)
- 57Gre: J. Greenspan, "Strengthening of Beryllium for High-Temperature Use by Means of Beryllium Oxide and Beryllium Carbide Dispersions," U.S. At. Energy Comm. TID-7526 (pt. 1), 34-53 (1957). (Equi Diagram; Experimental)
- 58Pas: P. Pascal, New Trait in Mineral Chemistry, 4, 102-131, Masson, Paris (1958) in French. (Equi Diagram; Review)
- *59Pol: B.D. Pollock, "Dissociation Pressure and Stability of Beryllium Carbide," J. Phys. Chem., 63(4), 587-589 (1959). (Equi Diagram, Thermo; Experimental)
- 60Bea: W.W. Beaver and D.W. Lillie, "Beryllium Metal, Alloys, and Compounds," Reactor Handbook, Interscience Publishers Inc., New York, 897-942 (1960). (Equi Diagram; Review)
- 63Fra: W.A. Frad, "Carbides," U.S. At. Energy Comm. IS-722, 94pp (1963). (Equi Diagram; Review)
- 63Sch: W. Schreiter, "Seltene Metalle, Rare Metals," Seltene Metalle, Rare Metals 1, 2nd ed., 343pp (1963) Verlag Grundstoffind, Leipzig. (Equi Diagram; Review)

- 64Eve: D.A. Everest, "Simple Binary Compounds of Be," in The Chemistry of Beryllium, Elsevier, Amsterdam, 82-90 (1964). (Equi Diagram; Review)
- 64Mot: K. Motzfeldt, "Equilibrium of the Reaction between Beryllium Oxide and Carbon to Give Beryllium Carbide," Acta Chem. Scand., **18**(2), 495-503 (1964). (Thermo; Experimental)
- 65Mol: G. Mollenstedt, H. Pollak, and H. Seiler, "Transformation of Beryllium into Be_2C and BeO by Electron Bombardment in the Presence of Hydrocarbon Polymers," Z. Phys., **182**, 445-450 (1965) in German. (Equi Diagram; Experimental)
- 66Mat: N.N. Matyushenko, A.A. Rozen, and N.S. Pugachev, "Triangulation of the System C-Si-Be," Porosh. Met., **6**, 61 (1966) in Russian; TR: Sov. Powder Met. Metal Ceram., **6**(4), 61-64 (1966). (Crys Structure; Experimental)
- 68Bla: R.O.G. Blachnik, P. Gross, and C. Hayman, "Heats of Formation of the Carbides of Aluminum and Beryllium," U.S. Clearinghouse Fed. Sci. Tech. Inform. AD 673897, 28pp (1968). (Thermo; Experimental)
- *70Bla: R.O.G. Blachnik, P. Gross, and C. Hayman, "Enthalpies of Formation of the Carbides of Aluminum and Beryllium," Trans. Faraday Soc., **66**, 1058-1064 (1970). (Thermo; Experimental)
- 70Cha: Y. Chabre and E. Geissler, "Self Diffusion in Beryllium Metal," Scripta Met., **4**, 255-257 (1970). (Equi Diagram; Experimental)
- 72Ald: F. Aldinger, "Effect of Hydrogen, Carbon, Nitrogen and Oxygen on the Properties of Beryllium," Metall., **26**(7), 711-718 (1972) in German. (Equi Diagram; Review)
- 73Fer: R. Ferro, "Crystal Structure and Density Data," in Beryllium: Physico-Chemical Properties of Its Compounds and Alloys, Atomic Energy Review: Special Issues, No. 4, 63-103, (ed.) O. Kubaschewski, UNIPUB, New York (1973). (Equi Diagram; Review)
- 73Gol: O. Von Goldbeck, "Phase Diagrams" in Beryllium: Physico-Chemical Properties of Its Compounds and Alloys, Atomic Energy Review: Special Issues, No. 4, 45-61, (ed.) O. Kubaschewski, UNIPUB, New York (1973). (Equi Diagram; Review)
- 80Kat: D.A. Katskov and I.L. Grinshtein, "Study of the Evaporation of Beryllium, Magnesium, Calcium, Strontium, Barium, and Aluminum from a Graphite Surface by an Atomic-Absorption Method," Zh. Prikl. Spektrosk., **33**(6), 1004-1012 (1980) in Russian. (Thermo; Experimental)
- 86BAP: to be published in Bull. Alloy Phase Diagrams (1986). (Equi Diagram; Compilation)

* Indicates key paper.

General References

- Hansen: M. Hansen and K. Anderko, Constitution of Binary Alloys, McGraw-Hill, New York or General Electric Co., Business Growth Services, Schenectady, NY 12345 (1958)
- Elliott: R.P. Elliott, Constitution of Binary Alloys, First Supplement, McGraw-Hill, New York or General Electric Co., Business Growth Services, Schenectady, NY 12345 (1965)
- Shunk: F.A. Shunk, Constitution of Binary Alloys, Second Supplement, McGraw-Hill, New York or General Electric Co., Business Growth Services, Schenectady, NY 12345 (1969)
- Pearson: W.B. Pearson, Handbook of Lattice Spacings and Structures of Metals and Alloys, Vol. 1 (1958) and Vol. 2 (1967), Pergamon Press, New York
- Landolt: Landolt-Bornstein Tables, New Series, Group III, Structure Data of Elements and Intermetallic Compounds, Springer-Verlag, New York (1971)
- Hultgren,E: R. Hultgren, P.D. Desai, D.T. Hawkins, M. Gleiser, K.K. Kelley, and D.D. Wagman, Selected Values of the Thermodynamic Properties of the Elements, American Society for Metals, Metals Park, OH (1973)
- Hultgren,B: R. Hultgren, P.D. Desai, D.T. Hawkins, M. Gleiser, and K.K. Kelley, Selected Values of the Thermodynamic Properties of Binary Alloys, American Society for Metals, Metals Park, OH (1973)
- Melt: "Melting Points of the Elements", Bull. Alloy Phase Diagrams, 2(1), 145-146 (1981)
- King1: H.W. King, "Crystal Structures of the Elements at 25 °C, Bull. Alloy Phase Diagrams, 2(3), 401-402 (1981)
- King2: H.W. King, "Temperature-Dependent Allotropic Structures of the Elements", Bull. Alloy Phase Diagrams, 3(2), 275-276 (1982)

Acknowledgments

Be-C evaluation contributed by L.E. Tanner, L-217, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550 and H. Okamoto, B77G, Lawrence Berkeley Laboratory, Berkeley, CA 94720. This work was supported by the U.S. Department of Energy under contract no. W-7405-Eng-48 and American Society for Metals (ASM). Literature searched through 1985. Part of the bibliographic search was provided by ASM. L.E. Tanner and H. Okamoto are ASM/NBS Data Program Category Editors for binary beryllium alloys.

Table 1 Be-C Crystal Structure and Lattice Parameter Data

Phase	Composition, at.% C	Pearson symbol	Struktur- bericht designation	Space group	Proto- type	Lattice parameters, nm		Reference
						a	c	
(β Be).....	0	cI2	A2	Im3m	W	0.25515	...	[King2]
(α Be).....	0	hP2	A3	P6 ₃ /mmc	Mg	0.22857	0.35839	[King1]
Be ₂ C.....	33.3	cF12	C1	Fm3m	CaF ₂	0.43420 \pm 5	...	[56Sta]
BeC ₂ (?)...	66.7	?	?	?	?	?	?	[24Dur]
(C).....	100	hP4	A9	P6 ₃ /mmc	graphite	0.24612	0.67090	[King1]